Torsion 114 O=[C:1][NX3H1:2]!@;-[c:3]([cH,nX2H0])[cH,nX2H0:4] 0.05 **Binned Counts** Fit **ETKDG Fit** 0.04 Probability per 10° Bin 0.03 0.02 0.01 0.00 60 120 180 Torsion (°)